

Journal of Magnetic Resonance

EDITOR : Wallace S. Brey, Jr.

EDITORIAL BOARD :

E. Raymond Andrew	David M. Grant	Ralph Livingston
Edwin D. Becker	R. K. Harris	Bruce McGarvey
A. David Buckingham	K. H. Hausser	Rex E. Richards
S. M. Castellano	Paul S. Hubbard	Max T. Rogers
B. P. Dailey	Charles S. Johnson, Jr.	Thomas A. Scott
P. Diehl	J. Jonas	Bernard L. Shapiro
Richard Ernst	Masaji Kubo	J. B. Stothers
Ray Freeman	George C. Levy	Robert L. Vold

Volume 24, 1976



ACADEMIC PRESS
New York and London

A Subsidiary of Harcourt Brace Jovanovich, Publishers

Copyright © 1976 by Academic Press, Inc.

ALL RIGHTS RESERVED

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

Made in Great Britain

CONTENTS OF VOLUME 24

NUMBER 1, OCTOBER 1976

B. N. MISRA AND S. D. SHARMA. ESR Hyperfine Linewidth and Bonding Parameter Studies of Cu(II) Complexes	1
RYUICHI IKEDA, YOSHIO KUME, DAIYU NAKAMURA, YOSHIHIRO FURUKAWA, AND HIDEKO KIRIYAMA. Motion of Methylammonium Ions in Methylammonium Hexachloroplatinate(IV) and Hexachlorostannate(IV) as Studied by Proton Magnetic Resonance	9
A. W. JOHNSON. Modulation Broadening of Second-Derivative Gaussian and Lorentzian Lines	21
DALLAS L. RABENSTEIN AND THOMAS L. SAYER. Carbon-13 Chemical Shift Parameters for Amines, Carboxylic Acids, and Amino Acids	27
THOMAS B. MARRIOTT, SHUI PONG VAN, AND O. HAYES GRIFFITH. Axial Isomer and ESR Spectra of the Steroid Spin Label, 3-Doxyl-5 α -Cholestane	41
AKIRA NAITO, KAZUYUKI AKASAKA, AND HIROYUKI HATANO. ENDOR Studies of γ -Irradiated L-Cystine Dihydrochloride. The Hyperfine Tensors from CH ₂ Protons in the Anion and the Cation	53
CHARLES S. JOHNSON, JR. The Effect of Torsional Vibrations on the Minimum Value of T_1 for Methyl Protons in Solids	63
D. I. HOULT AND R. E. RICHARDS. The Signal-to-Noise Ratio of the Nuclear Magnetic Resonance Experiment	71
N. C. BAIRD AND K. C. TEO. Effective Excitation Energies in ¹³ C NMR Chemical Shift Calculations	87
WILLIAM MCFARLANE AND DAVID S. RYCROFT. The Presentation of Nuclear Magnetic Triple-Resonance Spectra: A Study of the [(CH ₃ O) ₃ P] ₄ Cu ⁺ Cation by the MINDOR and the TINDOR Techniques	95
A. A. V. GIBSON, R. GOC, AND T. A. SCOTT. Lineshape and Temperature Dependence of the Nuclear Quadrupole Resonance of ¹⁴ N ₂ in β -Quinone Clathrate	103
C. A. McDOWELL, P. RAGHUNATHAN, AND D. S. WILLIAMS. Proton Magnetic Resonance and Relaxation in Solid Tertiary Butyl Amine-Tropolone Adduct	113
F. W. WARNER AND A. J. MCPHATE. A Combined Polynomial Regression and Nonderivative Search Technique for EPR Spectrum Analysis	125
P. A. NARAYANA AND LARRY KEVAN. Solution ENDOR of the Tri-t-butyl Phenoxy Radical: Nuclear Relaxation Mechanisms	137

G. VOIGT AND R. KIMMICH. Quadrupolar Dip in Proton Relaxation Dispersion of Poly(vinyl chloride)	149
THOMAS A. GERKEN AND WILLIAM M. RITCHEY. Lanthanide-Induced Proton, Carbon, and Phosphorus NMR Shifts for a Series of Organophosphorus Compounds	155

COMMUNICATIONS

ROBERT G. C. MCELROY AND ROBIN L. ARMSTRONG. Pure Nuclear Quadrupole Resonance Spectroscopy of Rubidium Hexabromoplatinate	165
SOON SAM KIM AND S. I. WEISSMAN. Detection of Transient Electron Paramagnetic Resonance	167

BOOK REVIEW

"Advances in Magnetic Resonance, Volume 8." Edited by John S. Waugh	171
---	-----

NUMBER 2, NOVEMBER 1976

JENS PETER JACOBSEN AND KJELD SCHAUMBURG. Spin-Lattice Relaxation Time Measurements of D ₂ O in a Lyotropic Phase	173
THOMAS K. LEIPERT AND DONALD W. MARQUARDT. Statistical Analysis of NMR Spin-Lattice Relaxation Times	181
ANTONIO DE MARCO AND KURT WÜTHRICH. Digital Filtering with a Sinusoidal Window Function: An Alternative Technique for Resolution Enhancement in FT NMR	201
ROBERT N. SCHWARTZ. Relaxation of Spin- $\frac{1}{2}$ Nuclei of Heavy Atoms in Electrolyte Solutions	205
G. KRISHNAMOORTHY AND B. S. PRABHANANDA. Study of Molecular Motions in Liquids by ESR and Relaxation Measurements. III. Temperature Dependence of <i>g</i> of Semiquinones in Alcohols	215
K. RAMANI, S. GANAPATHY, AND R. SRINIVASAN. A Fourier Transform Approach to Voigt Profile Analysis and Its Application to Nuclear Magnetic Resonance	231
C. C. HINCKLEY AND W. C. BRUMLEY. Errors in Analyses of Lanthanide-Induced Shifts. <i>Cis</i> - and <i>Trans</i> -Pinocarveol	239
GARY E. MACIEL AND HARRY C. DORN. Approximate SCF Perturbation Theory of ¹³ C Chemical Shifts. Compounds Containing Nitrogen	251
A. R. BOATE, J. R. MORTON, AND K. F. PRESTON. Analysis of ESR Spectra of Radicals Having Large Hyperfine Interactions	259
R. J. C. BROWN, J. G. SMELTZER, AND R. D. HEYDING. Nuclear Quadrupole Resonance and Thermal Expansion in Perrhenate Salts	269

V. A. CHERTKOV, YU. K. GRISHIN, AND N. M. SERGEYEV. Proton-Coupled ^{13}C NMR Spectra of Cyclopentadiene	275
---	-----

COMMUNICATIONS

JOHN D. GRAHAM AND JEROME S. DARBY. Spin-Lattice Relaxation Times of Individual Dilute ^{13}C Nuclei in Crystals	287
---	-----

GEOFFREY BODENHAUSEN, RAY FREEMAN, REINHARD NIEDERMEYER, AND DAVID L. TURNER. High Resolution NMR in Inhomogeneous Magnetic Fields	291
--	-----

R. KAPTEIN, K. DIJKSTRA, AND C. E. TARR. A Single-Scan Fourier Transform Method for Measuring Spin-Lattice Relaxation Times	295
---	-----

BOOK REVIEW

"Spin Labeling, Theory and Applications." Edited by Lawrence J. Berliner	301
--	-----

ANNOUNCEMENTS AND NEWS ITEMS	303
--	-----

PAPERS TO APPEAR IN FUTURE ISSUES	305
---	-----

NUMBER 3, DECEMBER 1976

V. A. LIVSHITS. Slow Anisotropic Tumbling in ESR Spectra of Nitroxyl Radicals	307
---	-----

MASAHIRO KONDO, ISAO ANDO, RIICHIRO CHÛJÔ, AND ATSUO NISHIOKA. Theoretical Calculation of Carbon-13 NMR Shielding Constants and Their Tensors in Hydrocarbons by the Finite Perturbation Method	315
---	-----

W. M. M. J. BOVÉE. Longitudinal and Transverse NMR Relaxation in a Proton AB System	327
---	-----

YVES SERVANT, JEAN-CLAUDE BISSEY, AND SLIMANE GHARBAGE. X-Band ESR Faraday and Cotton-Mouton-Voigt Effects of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ and $\text{Cu}(\text{NH}_4\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ in Polycrystalline Powder	335
---	-----

A. KALK AND H. J. C. BERENDSEN. Proton Magnetic Relaxation and Spin Diffusion in Proteins	343
---	-----

J. C. MACDONALD AND M. MAZUREK. Carbon-13 Spectra: Some Effects of Radiofrequency Amplitude in Proton-Spin Decoupling	367
---	-----

GEORGE C. LEVY, ULF EDLUND, AND CLIVE E. HOLLOWAY. Mechanisms for Interactions between Organic Molecules and Paramagnetic Relaxation Reagents	375
---	-----

E. W. STOUT, JR. AND H. S. GUTOWSKY. On the Temperature Dependence of Lanthanide-Induced NMR Shifts.	389
--	-----

H. E. SIMON AND R. L. VOLD. Proton Relaxation and Molecular Motion in Binary Liquid Mixtures	399
ADAM ZIPP, IRWIN D. KUNTZ, AND THOMAS L. JAMES. An Investigation of "Bound" Water in Frozen Erythrocytes by Proton Magnetic Resonance Spin-Lattice, Spin-Spin, and Rotating Frame Spin-Lattice Relaxation Time Measurements	411
ANIL KUMAR AND RICHARD R. ERNST. Influence of Nonresonant Nuclei on NMR Spin Echoes in Liquids and in Solids	425
R. K. HARRIS AND R. H. NEWMAN. Choice of Pulse Spacings for Accurate T_1 and NOE Measurements in NMR Spectroscopy	449
COMMUNICATIONS	
P. GONORD, S. K. KAN, AND M. SAUZADE. FT Interpolation of NMR Spectral Segments	457
RAJ K. GUPTA. Dynamic Range Problem in Fourier Transform NMR. Modified WEFT Pulse Sequence	461
D. L. VANDERHART. Observation of Natural Abundance, ^{13}C - ^{13}C Dipolar Satellites in Ultraoriented Polyethylene	467
BOOK REVIEW	
"NMR Basic Principles and Progress. Volume 9: Lyotropic Liquid Crystals," by C. L. Khetrapal, A. C. Kunwar, A. S. Tracey, and P. Diehl.	471
AUTHOR INDEX FOR VOLUME 24	473
SUBJECT INDEX FOR VOLUMES 21-24	475

Information for Authors

The *Journal of Magnetic Resonance* includes original papers, both full articles and communications, dealing with the theory, techniques, methods or spectral analysis and interpretation, spectral correlations, and results of magnetic resonance spectroscopy and related fields. Submission of a manuscript to the *Journal* implies that none of the content has been published or is under consideration for publication elsewhere, except as specifically indicated by the author. The Editor seeks the assistance of expert referees in the evaluation of manuscripts of articles, but he alone is responsible for the final decision concerning acceptance.

Communications are preliminary accounts of work of special importance or contain discussion of controversial subjects. Communications must be especially carefully and concisely prepared; since they may not be refereed, it is the responsibility of the author to ensure that the manuscript as originally submitted is free of typographical or substantive errors. To save time in publication, proofs of communications are not sent to the authors for correction.

Fifty reprints of each paper are supplied without charge, and additional reprints may be ordered on a form which is sent to the author. For articles, the reprint order form accompanies the galley proofs which the author receives. The *Journal assesses no page or publication charges*.

All manuscripts and books for review should be sent to the Editor, Wallace S. Brey, Department of Chemistry, University of Florida, Gainesville, Florida 32611.

Arrangement of the Paper

If the paper is lengthy, it should be divided into sections, although it is preferred that the sections not be numbered. Tables are numbered consecutively with *Arabic* numerals and are to be mentioned in order in the text. Each table should be supplied with a title. Figures are also numbered consecutively with *Arabic* numerals and are mentioned in order in the text. Each regular article requires an abstract which should describe concisely the substantive content, the conclusions reached, and the contributions of the research described. Since the abstract may be used directly by Chemical Abstracts and other abstracting services, it must be self-contained, having no references to formulas, equations, or bibliographic citations which appear in the body of the manuscript.

Literature references are cited in numerical order in the text by *in-line, parenthesized, italic numerals*. References to "unpublished" or "to be published" work from the author's laboratory should not be given. However, dissertations may be cited, or papers actually accepted may be referred to as "in press" if the name of the journal is included.

Authors are urged to give careful thought to the logical construction of the manuscript, so that explanatory or parenthetical footnotes need not be employed—where possible, such material should be incorporated in the text. Any footnotes which are indispensable are not intermixed with references, but are indicated in the text by consecutive, superscript numerals, and each footnote will then appear in print at the bottom of the page on which it is cited. Equation numbers are given in *square* brackets to the right of the equation, and references in the text to equations should be in the form "Eq. [3]."

Form of Manuscript

Manuscripts should be submitted in triplicate. The *original typewritten copy* should be supplied; mimeo, electrostatic and similar process reproductions are not usually sufficiently clear. All of the typing must be *double-spaced*, including that of abstract, references, and footnotes, on one side of good quality paper approximately 22 × 28 cm (8.5 × 11 in.) in dimensions. The first line of each paragraph is indented.

Each page of the manuscript should be numbered. The first page contains the article title, the author's name, and affiliation. At the bottom of this page should appear any footnotes to the title (indicated by superscript *, †, ‡); the number of manuscript pages, figures, and tables should also be noted. The second page should contain the abstract of 50–200 words.

Symbols and Abbreviations. The American Chemical Society's Handbook for Authors, 1967 edition, or the Style Manual of the American Institute of Physics should be followed for standard abbreviations, names and symbols for units. Mathematical equations or symbols must be typewritten whenever possible. Greek letters may be identified in pencil in the margin. The author of any manuscript in

which there are mathematical equations or symbols is urged to supply a list of these on a separate sheet for the assistance of the printer in selecting the proper type. The list will not appear in print.

References and Footnotes. References to the literature should be cited in order in the text by in-line, parenthesized numerals. The references themselves are to be typed double-spaced on a separate sheet in numerical order. Each reference contains the author's initials, last name, journal name, volume, initial page number and year in parentheses, *in that order*. The name of the journal is abbreviated in the style of Chemical Abstracts' *Service Source Index* (1969 Edition). For book references, the form is author's name, name of the book in quotation marks, editor's name (if any), edition if other than the first, chapter or page number, publisher's name, place of publication, and year of publication.


Any footnotes which are included are numbered in a sequence separate from the references and must be typed in the manuscript on a separate page.

Tables. Tables should be laid out carefully, so that minimum space is used and entries are accurately grouped and clearly labeled. Usually, a table should be arranged vertically, with more rows than columns. Vertical lines are not used to separate the columns. Each table is numbered with an Arabic numeral, provided with a title, and typed on a separate sheet of paper. Footnotes to the table are placed directly below it and are indicated by superscript, lower-case, italic letters (^a, ^b, ^c). Tables that are longer than two manuscript pages will be reproduced photographically, and should therefore be typed in the exact form desired. All such tables should be carefully checked since errors cannot be corrected in proof.

Figures. Figures must be carefully drawn in black, waterproof drawing ink, to draftsman's standards, with lettering by stencil or drawing machine. Freehand, penciled, or typewritten lettering is not acceptable. Lettering should include numerical scales and units required for the two axes, and should be large enough to be legible after reduction by 50–60%. The illustration copy should be on sheets of the same size as that on which the manuscript is typed. Smaller figures may be mounted on sheets of the required size, and larger originals may be handled by supplying glossy, high-contrast, photographic reductions. The original and two duplicates of each figure are required.

Diagrams. Ink drawings should be supplied for any complex molecular formulas or diagrams involving material which the printer cannot readily set in type.

Proofs. Galley proofs will be sent to the author with reprint order forms. Fifty reprints of each article will be supplied free of charge.



Digitized by the Internet Archive
in 2023 with funding from
Kahle/Austin Foundation

